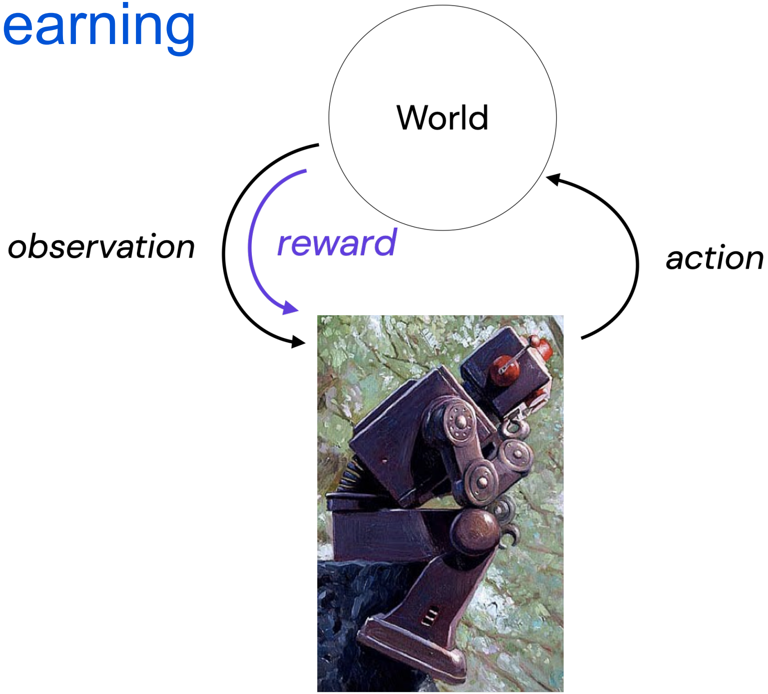
What is Reinforcement Learning for?

Reinforcement Learning



"Part of the appeal of reinforcement learning is that it is in a sense the whole AI problem in a microcosm."
– [Sutton, 1992]

1. RL for understanding intelligence

- A way to model processes in the brain
- A way to model cognitive processes in animals and people

Learning Values: Temporal-Difference Error

- Value estimate at time step *t*: $v(S_t)$
- Value estimate at time step *t+1*: $r(S_t, A_t) + \gamma v(S_{t+1})$
- *Temporal-difference error:*

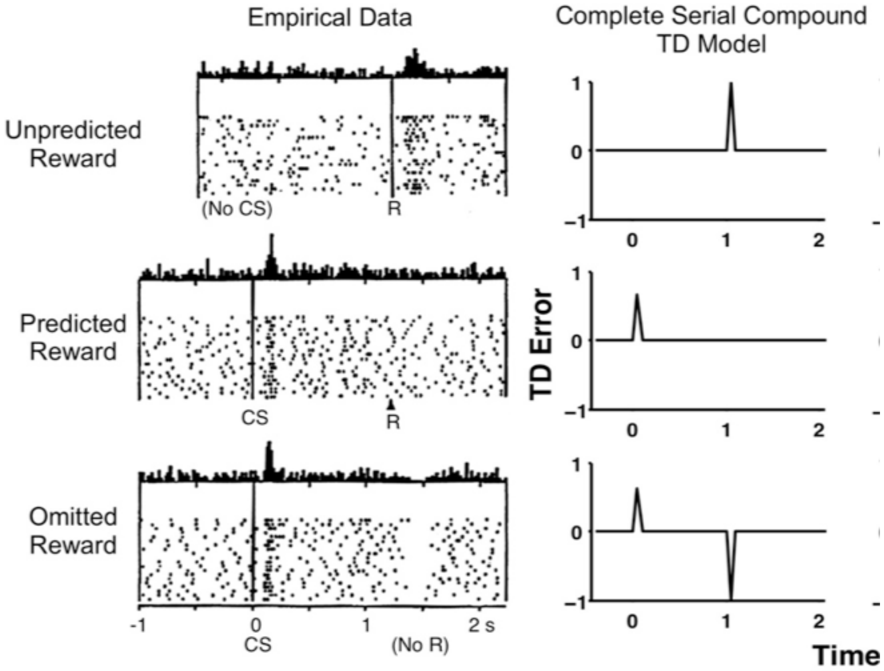
$$\delta_t = r(S_t, A_t) + \gamma v(S_{t+1}) - v(S_t)$$

- If v is parameterized by w, change w so as to minimize the TD-error:

$$\mathbf{w}_{t+1} = \mathbf{w}_t + \alpha \delta_t \nabla_{\mathbf{w}} v_{\mathbf{w}}(S_t)$$

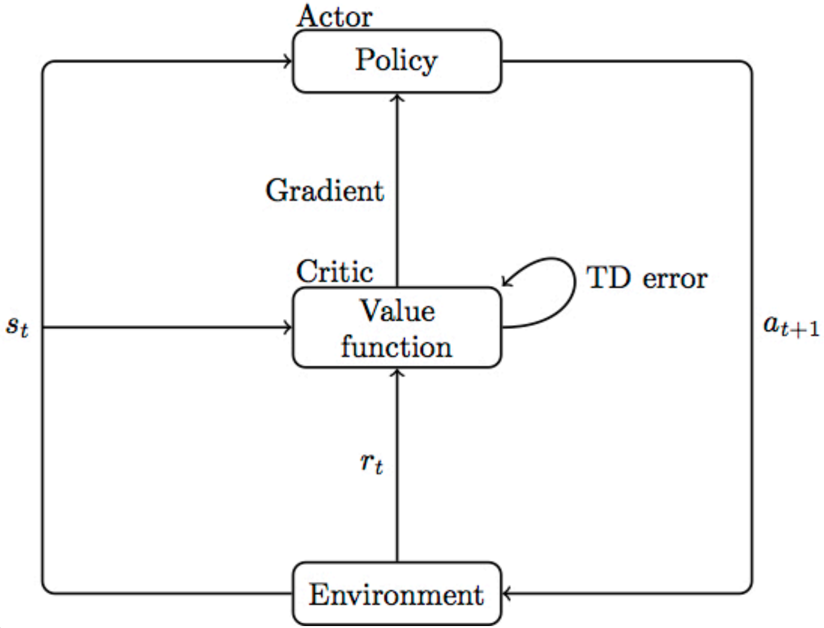
- Shultz, Dayan & Montague (1997): TD-errors model the activity of dopamine neurons

Dopamine neuron modelling



Cf. Shultz, Dayan et al, 1996; and lots of follow-up work including MNI, Psych.

Control: Actor-critic architecture



- Parameters of the policy move to make more likely action a that has positive advantage:

$$A(s,a) = r(s,a) + \gamma \mathbf{E}(v(s') \mid s,a) - v(s)$$

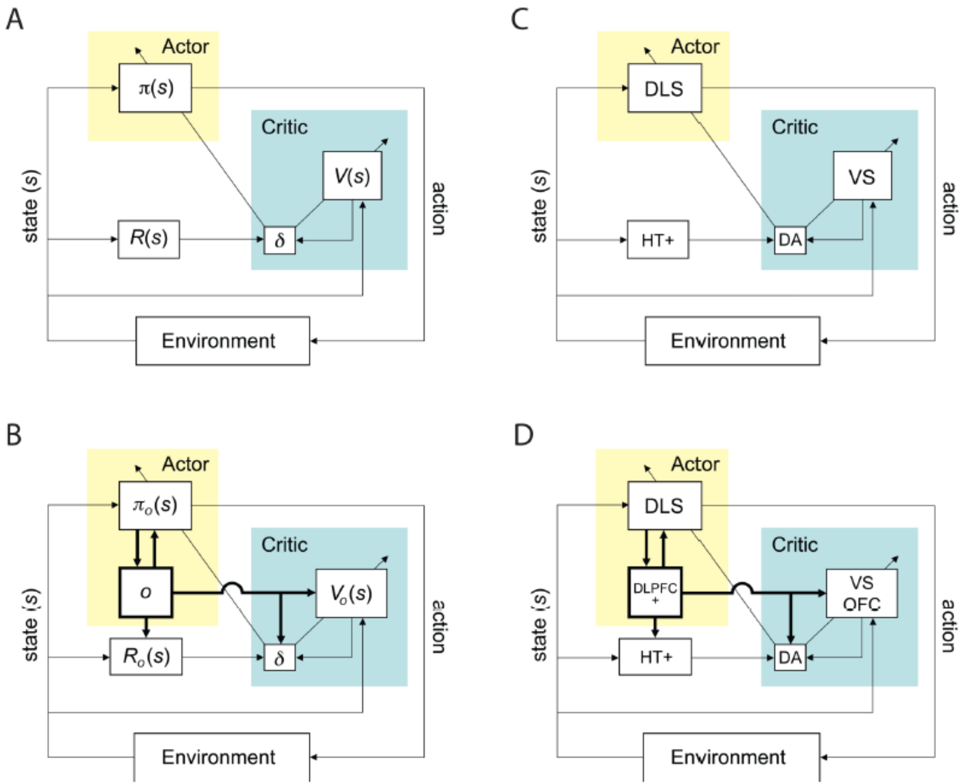
- O'Doherty et al (2004): fMRI evidence that dorsolateral striatum implements an actor and ventral striatum a critic

Generalizing Actions: Options Framework

- An *option* is a defined by a tuple $\langle I_\omega(s), \pi_\omega(a\,|\,s), \beta_\omega(s)\rangle$
  - An *initiation function* (precondition)
  - An *internal policy* (behavior)
  - A *termination function* (post-condition)
- Eg robot navigation: if no obstacle in front (initiation) go forward (policy) until something is too close (termination)

Cf. Sutton, Precup & Singh, 1998; Precup, 2000

Possible Neural Correlates of Options

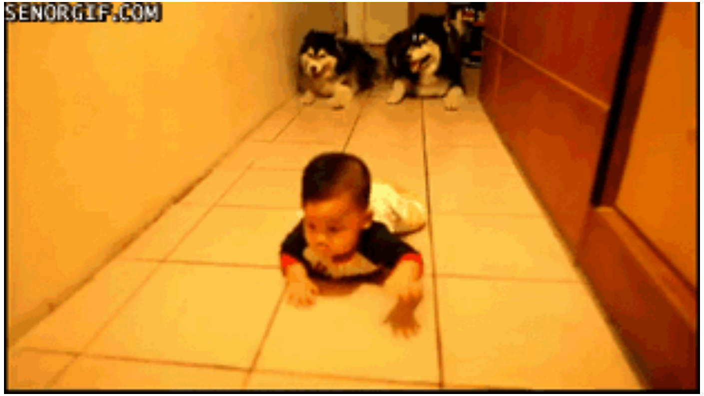


From Botvinick, Niv & Barto, 2009

“

Affordances […] relations between abilities of organisms and features of their environment.

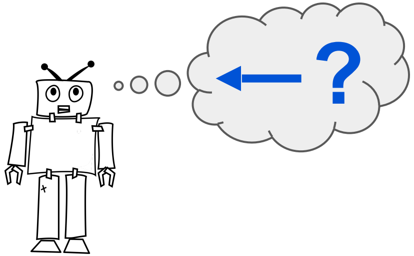
Gibson, 1977



Source: Giphy

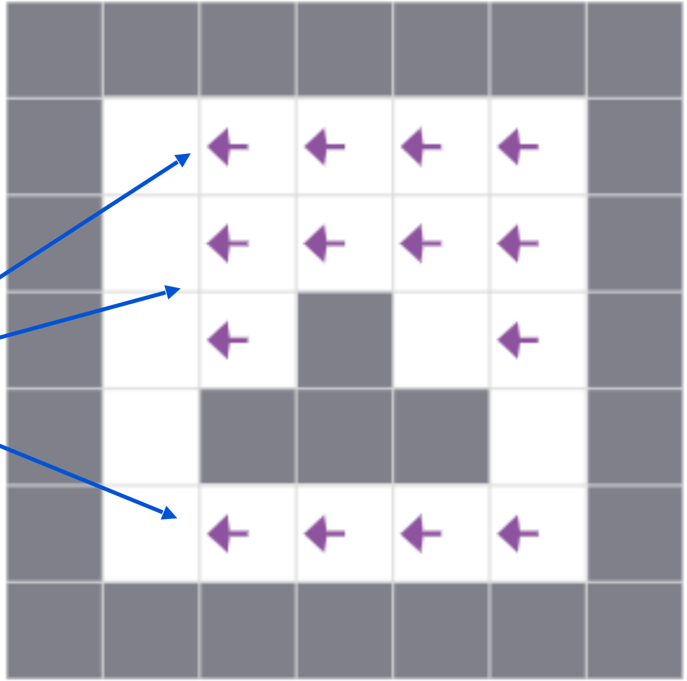
Affordances

- Captures states and actions that complete an intent



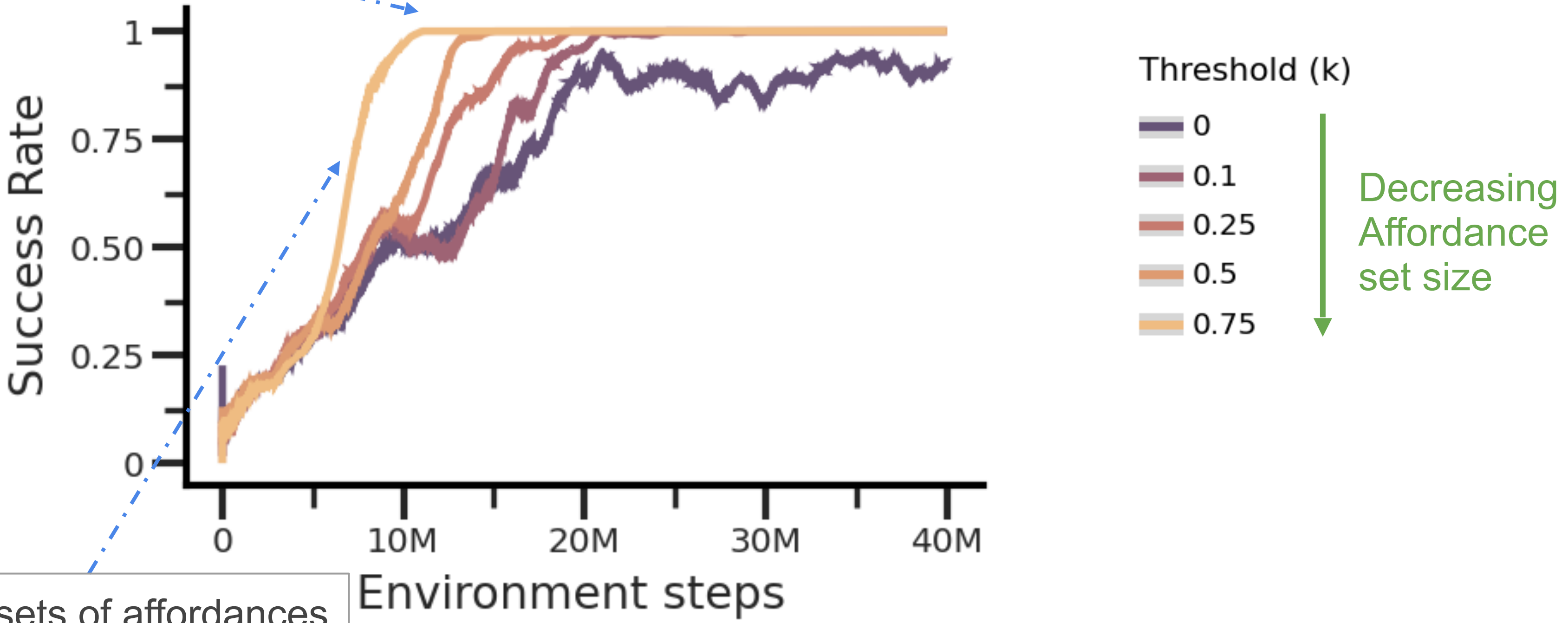
$$\mathcal{AF}_{\mathcal{I}} \subseteq \mathcal{S} \times \mathcal{A}$$

Affordances are the subset of states and actions which complete the intent to go left.



What is the impact of the affordance set size on performance ?

Performance gains



Smaller sets of affordances
= quicker learning

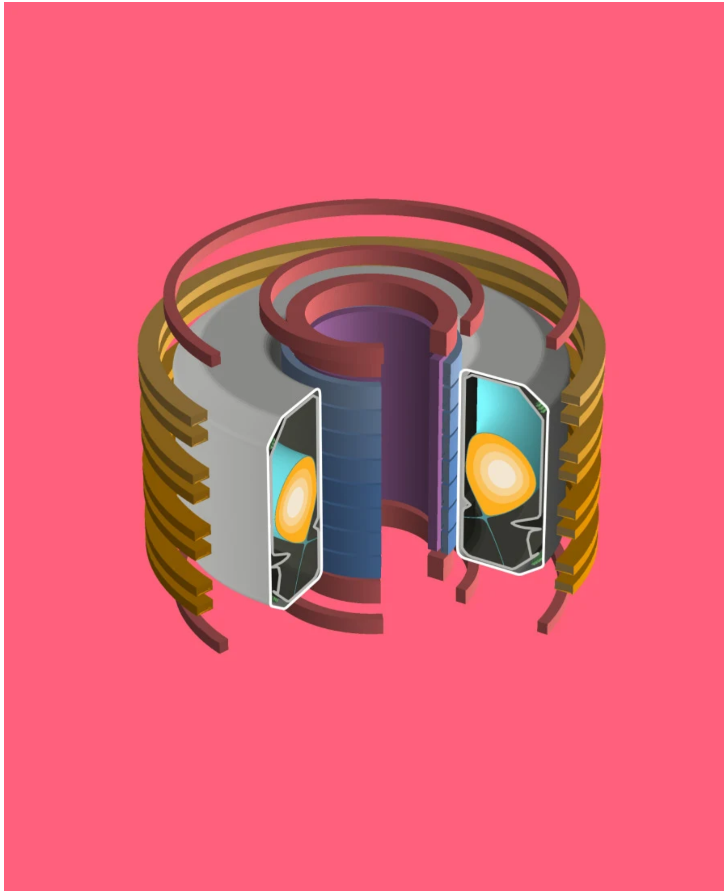
2. RL for applications

- Build (super-human) agents for language, games (discussed already)
- Tackle very complex control tasks
- Learn to search and explore

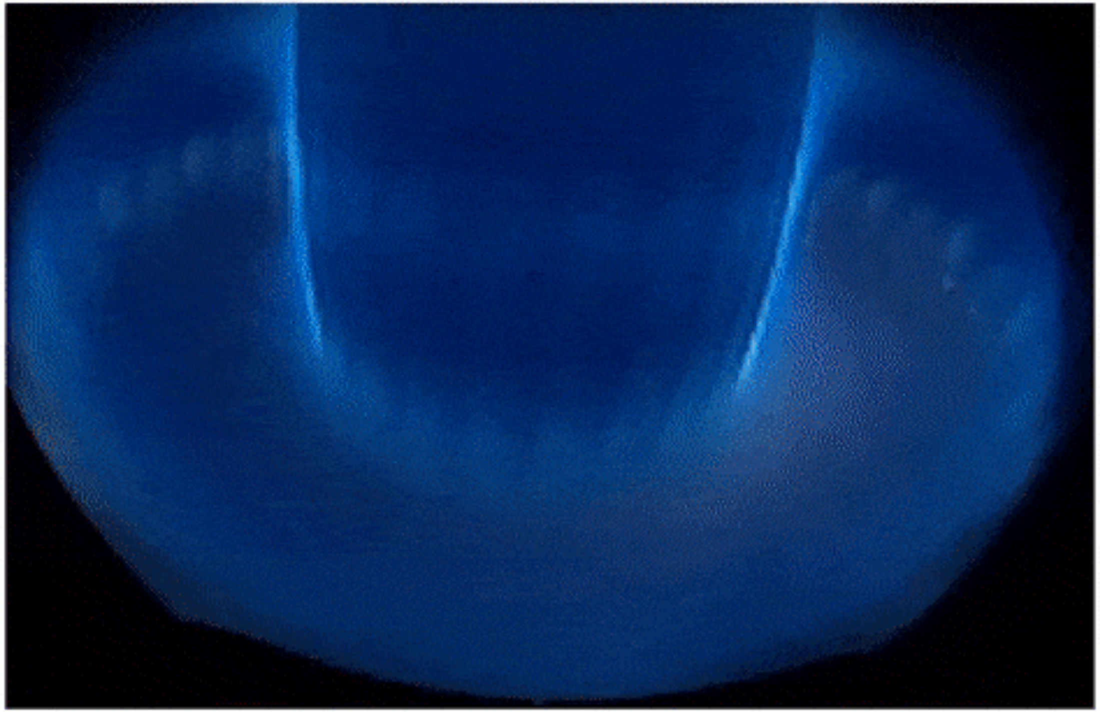
RL for controlling fusion reactors (Degrave et al, Nature 2022)

- Goal: achieve cheap clean energy!
- Tokamak reactor (EPFL): control 19 magnetic coils to get and maintain plasma into a specific shape
- True reward: energy output
- Proxy reward: penalize deviation from desired shape

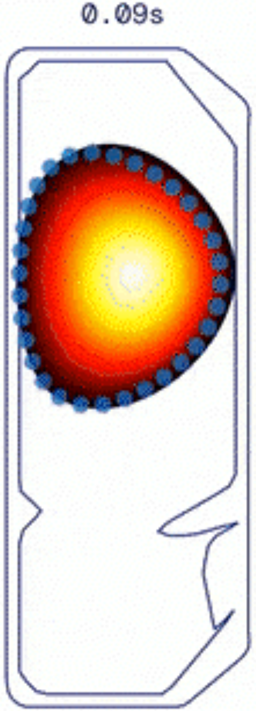
What does a Tokamak look like?



Inside a Tokamak reactor



View from inside the tokamak

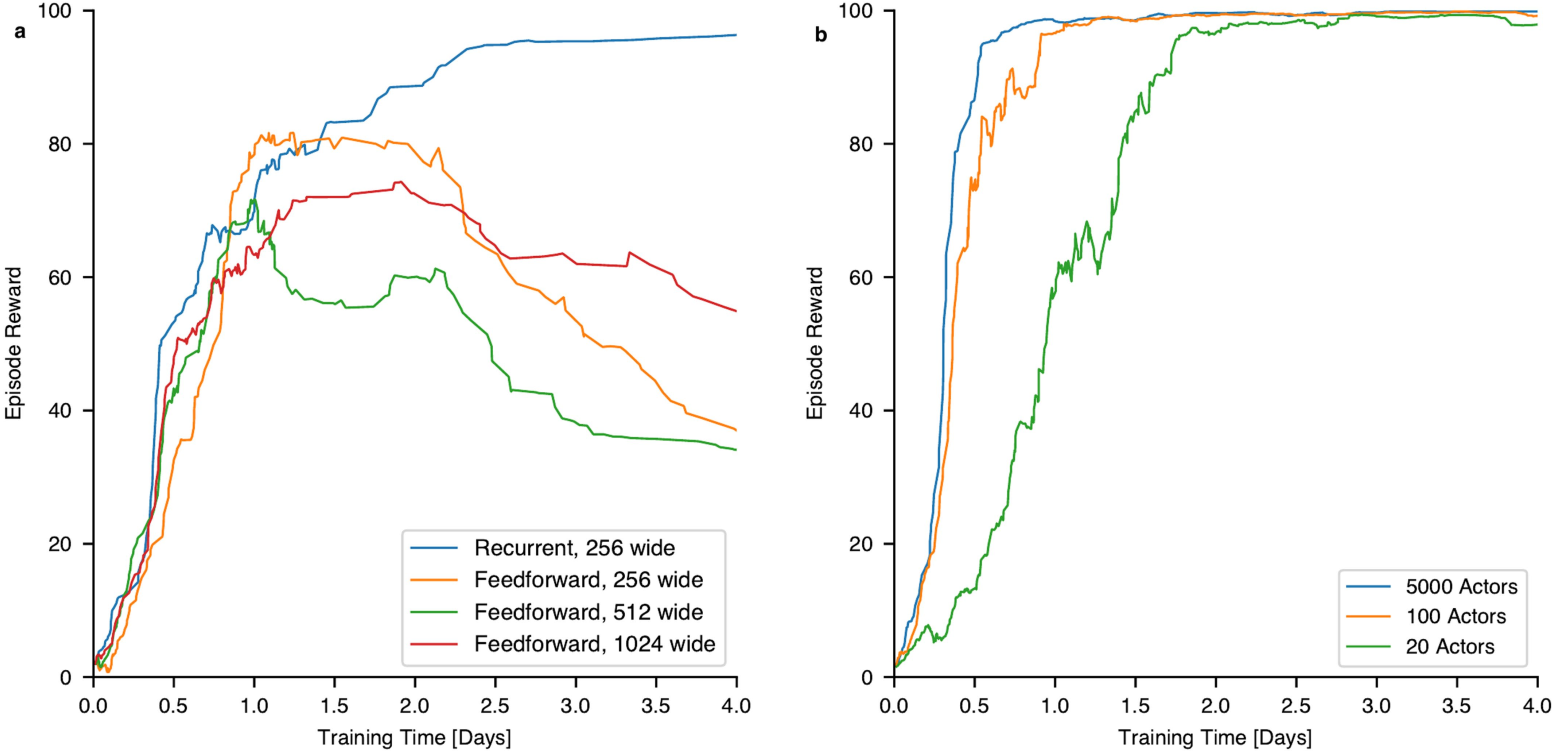


Plasma state reconstruction

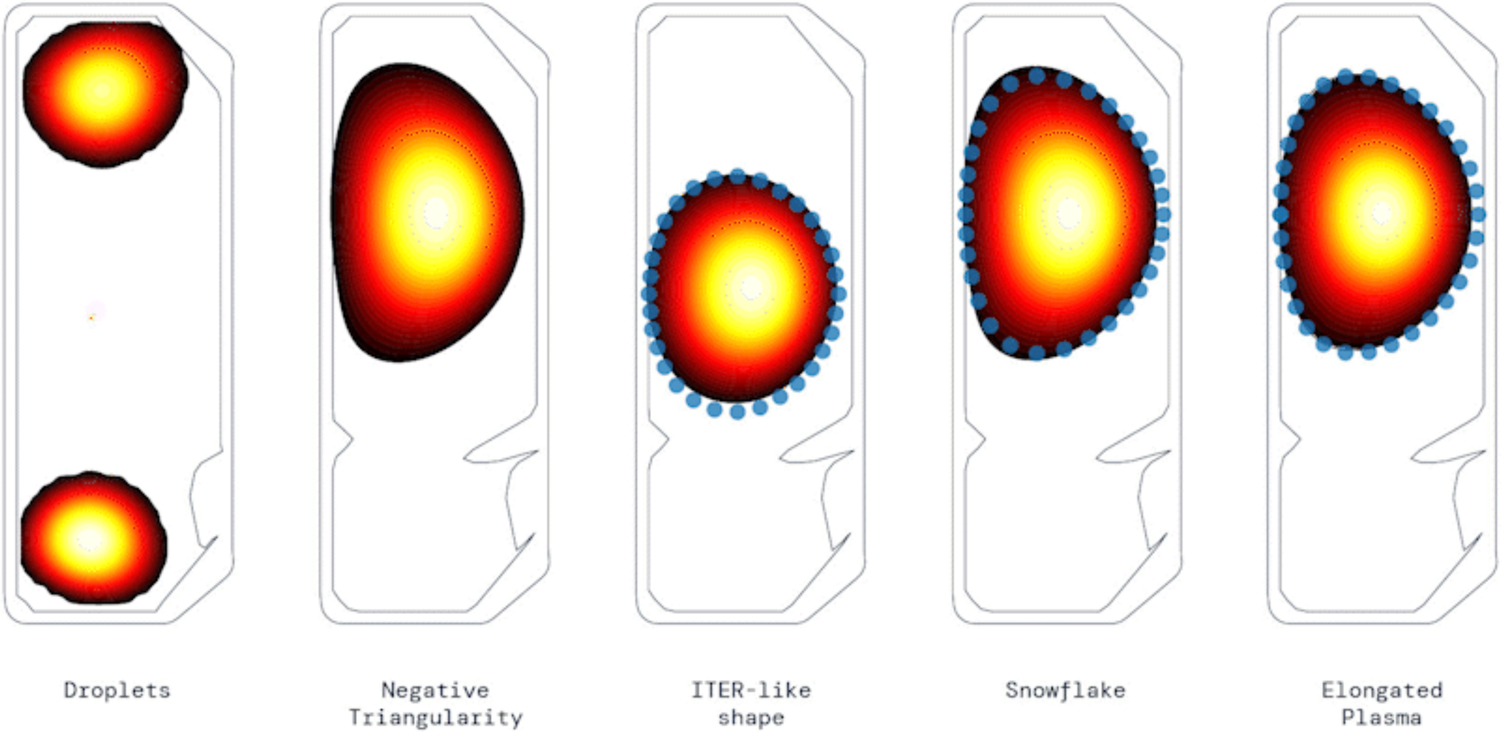
Recipe

- Build a simulator of the problem (using knowledge of physics
- Train an RL agent using policy optimization (MPO, Abdomaleki et al 2018)
- Take only the trained policy and deploy on a real reactor to evaluate
- Note control has to happen at 10kHz!

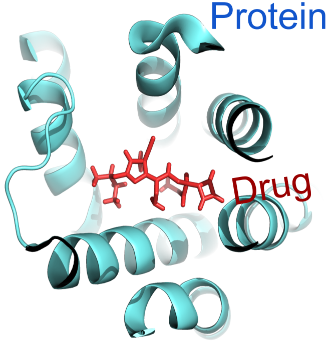
Quantitative results



Qualitative results

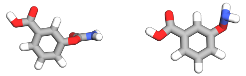


Small Molecule Drug Discovery



Initial data
{(*x*,*y*),..}

occasionally query “oracle"



generate molecule(s)

predict reward
cheaply (DNN)

compute “real” reward

growing
dataset

train reward
predictor

train
generator

This part is expensive and/
or noisy!
(w/ biased noise)

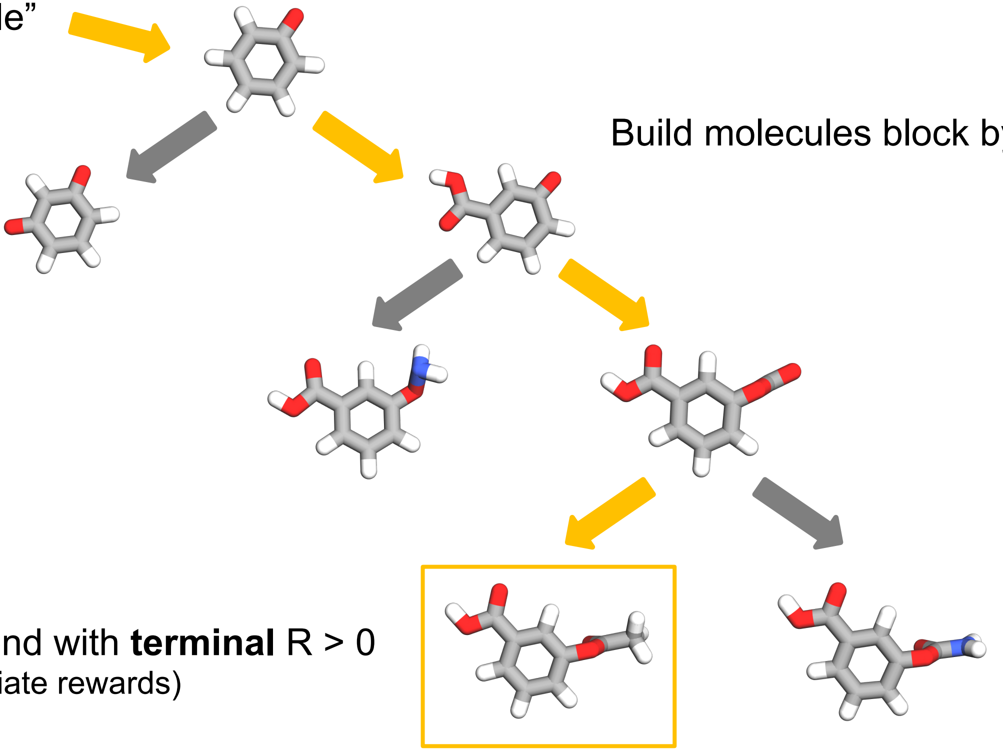
Oracle?

- Ideal: send **diverse** batches (10-100k) of candidates to a lab, O(weeks)
- For now: use noisy physics simulator, O(15 CPUs)/molecule

Drug Discovery as Reinforcement Learning Problem

“empty molecule”

Build molecules block by block



Episodes end with **terminal** R > 0
(no intermediate rewards)

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Just apply Reinforcement Learning?

- We have an environment (actions = build molecule)
- We have a (noisy, learned) reward
- RL! (Segler et al., 2017; De Cao & Kipf, 2018; Popova et al., 2019;
  Gottipati et al., 2020; Angermueller et al., 2020)

But RL greedily looks for one mode, even when we encourage entropy!
Not great for *diverse* batch oracle queries

What about the usual generative models?

- Trained from positive samples only (e.g. existing drugs)
  But we have a more informative (non-binary) signal! (reward)
- We don't just want high reward, we want to avoid low reward (and have the data)
- Still possible to do well: Jin et al., 2018; Shi et al., 2020; Luo et al., 2021

GFlowNet

Flow Network based Generative Models for Non-Iterative Diverse Candidate Generation

Emmanuel Bengio[1,2], **Moksh Jain**[1,5], **Maksym Korablyov**[1]
Doina Precup[1,2,4], **Yoshua Bengio**[1,3]
[1]Mila, [2]McGill University, [3]Université de Montréal, [4]DeepMind, [5]Microsoft

NeurIPS 2021

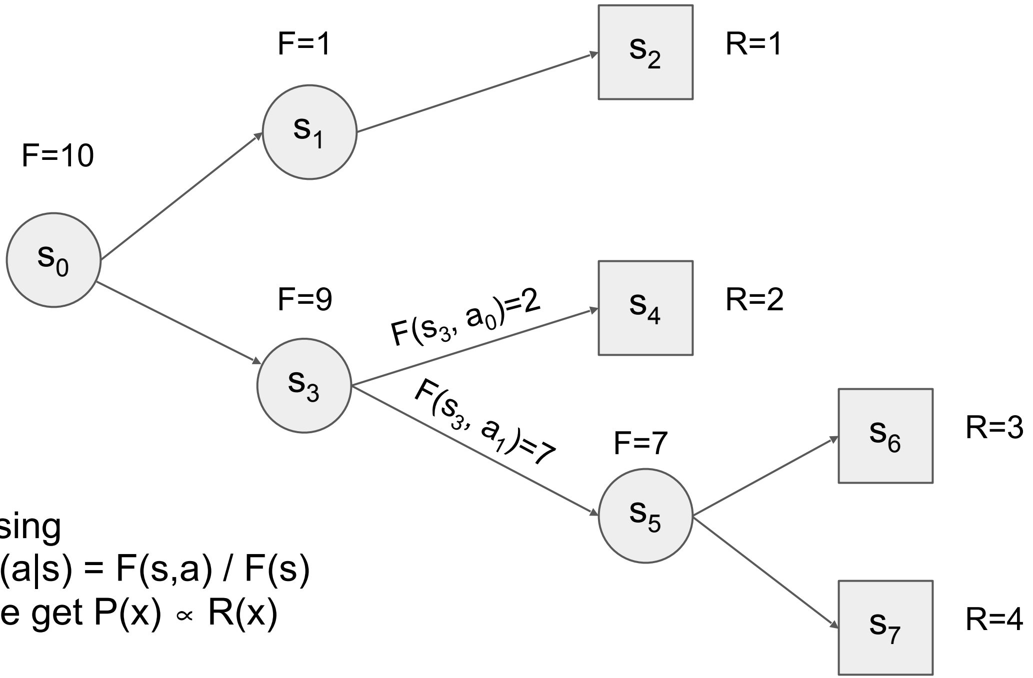
Generative framework for discrete objects which have a reward (or energy).

Desired: Reward-proportional sampling!

$$\pi(x) \approx \frac{R(x)}{Z} = \frac{R(x)}{\sum_{x' \in \mathcal{X}} R(x')}$$

Background: SumTrees (& control as inference: SoftAC/SoftQL)

$\pi(a|s) = Q(s,a) / V(s) = F(s,a) / F(s)$



$P(s_2)$ = 1/10

$P(s_4)$ = 2/10

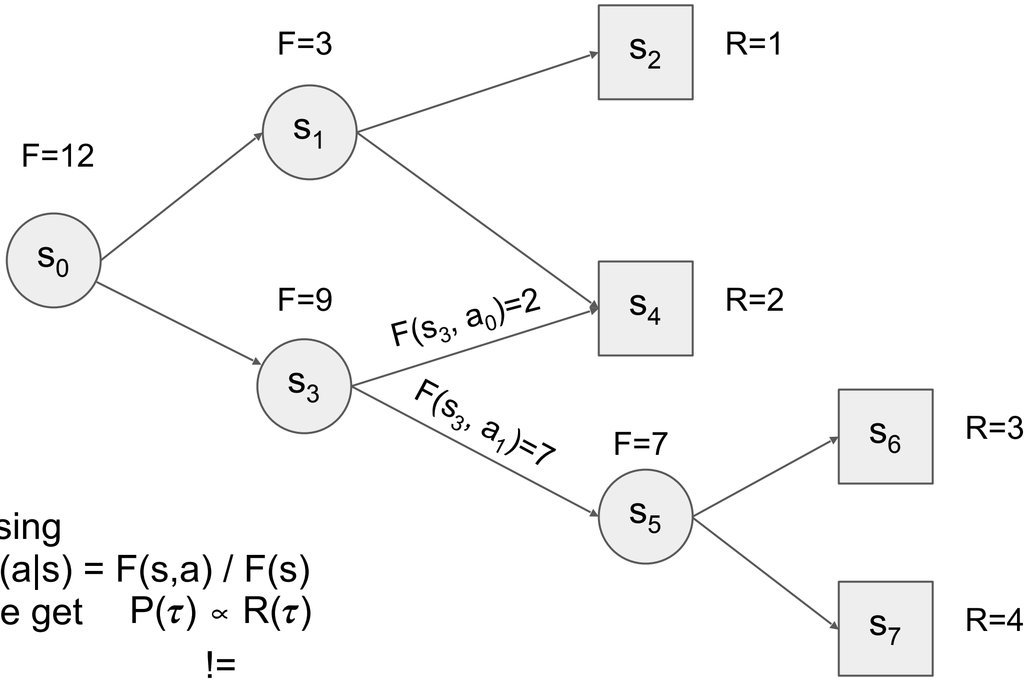
$P(s_6)$ = 3/10

$P(s_7)$ = 4/10

using
$\pi(a|s) = F(s,a) / F(s)$
we get $P(x) \propto R(x)$

What if it's a DAG?

Naively applying SoftQL/SumTree yields the wrong solution



$P(s_2) = 1/12$

$P(s_4) = 4/12$

$P(s_6) = 3/12$

$P(s_7) = 4/12$

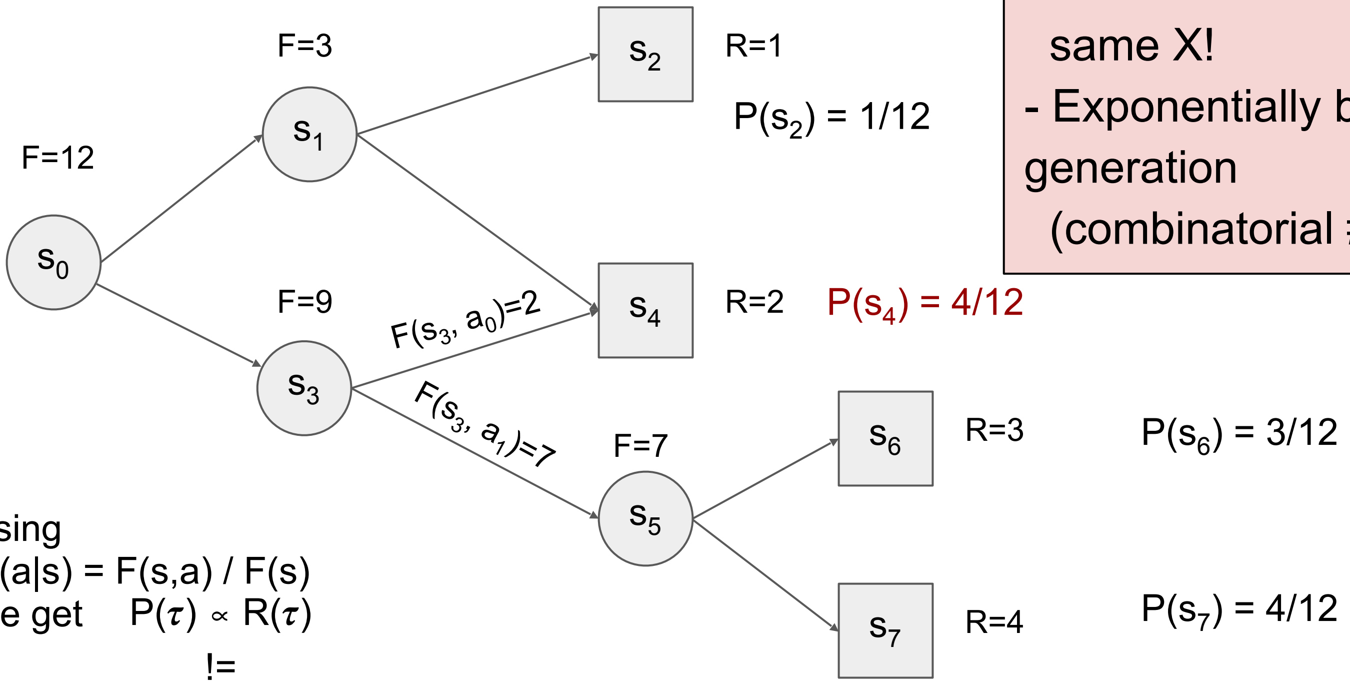
using
$\pi(a|s) = F(s,a) / F(s)$
we get $P(\tau) \propto R(\tau)$

!=

$P(x) \propto R(x)$

What if it's a DAG?

Naively applying SoftQL/SumTree yields the wrong solution



using
$\pi(a|s) = F(s,a) / F(s)$
we get $P(\tau) \propto R(\tau)$

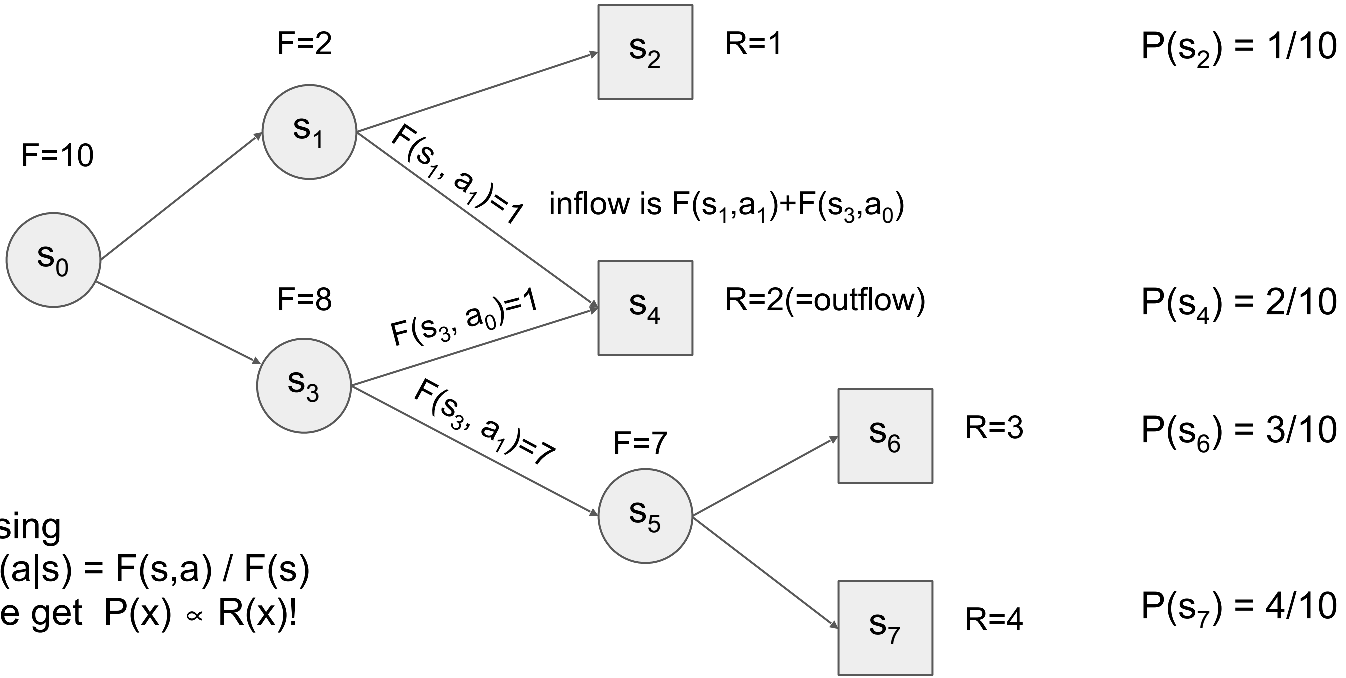
!=

$P(x) \propto R(x)$

- $P(\tau) \propto R(\tau)$ is bad if many τ lead to the same X!
- Exponentially bad in graph generation (combinatorial # of paths)

Interpreting the DAG as a flow network

F(s) such that inflow = outflow



using
$\pi(a|s) = F(s,a) / F(s)$
we get $P(x) \propto R(x)$!

Flow consistency

Satisfy flow conditions, for all s'

$$\sum_{s,a:T(s,a)=s'} F(s,a) = R(s') + \sum_{a' \in \mathcal{A}(s')} F(s',a')$$

in flow of s' out flow of s'

This is very similar to a Bellman Equation, the bread and butter of RL!

Satisfying the flow equations yields the right sampling proportions

How to train GFlowNet

Take inspiration from RL to learn *F:*

$$\tilde{\mathcal{L}}_\theta(\tau) = \sum_{s' \in \tau \neq s_0} \left(\sum_{s,a:T(s,a)=s'} F_\theta(s,a) - R(s') - \sum_{a' \in \mathcal{A}(s')} F_\theta(s',a') \right)^2$$

Dangerous objective, $F(s_0,.)$ is going to be huge! $F(s_0) = Z$

How to train GFlowNet

Instead, learn the log, **and** match flows in log-space

$$\mathcal{L}_{\theta,\epsilon}(\tau) = \sum_{s' \in \tau \neq s_0} \left(\log \left[\epsilon + \sum_{s,a:T(s,a)=s'} \exp F_\theta^{\log}(s,a) \right] - \log \left[\epsilon + R(s') + \sum_{a' \in \mathcal{A}(s')} \exp F_\theta^{\log}(s',a') \right] \right)^2$$

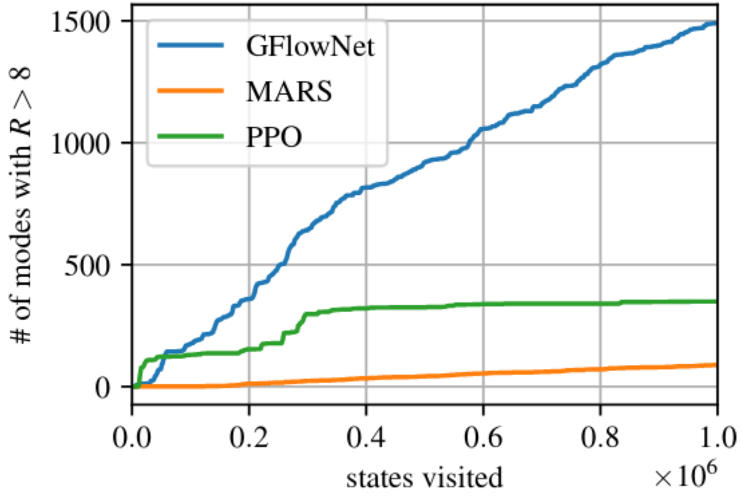
with an epsilon (care less about tiny flows)

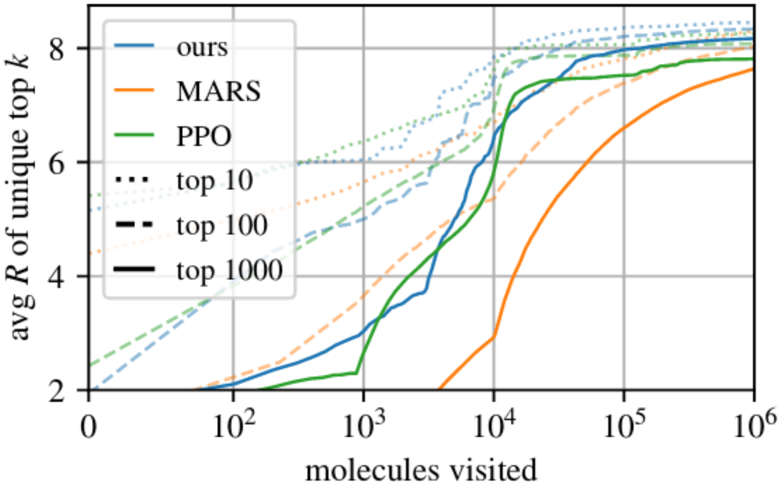
Relationship to MaxEntRL

- Quite similar in spirit but different mechanism (recent papers establish formal relationship)
- *Sampling of trajectories is always proportional to the reward at the end*
- If multiple policies are optimal their paths continue to be generated
- In fact, all paths continue to be generated
- Ongoing work: extensions to non-DAG, rewards at all states

Works well! Molecule results

Pre-train reward function once on 300k molecules (computed on CPU simulator)
Modes are found faster, with better rewards





modes = Bemis-Murcko scaffolds

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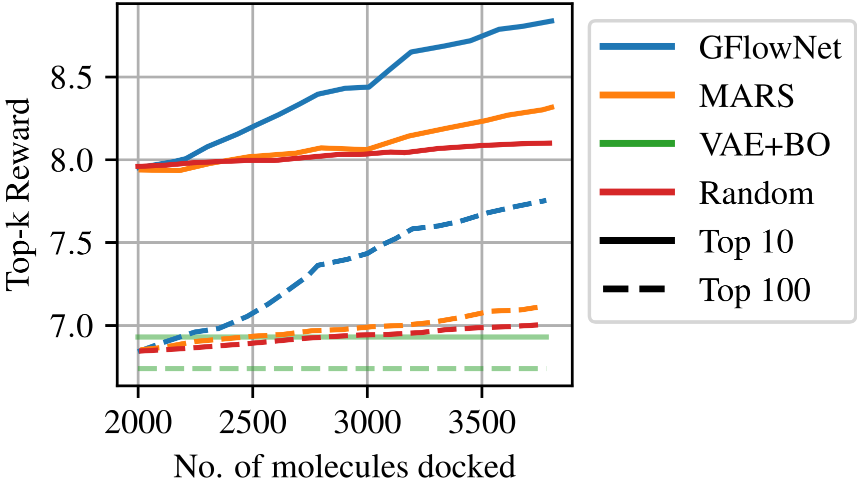
Works for Batch Active Learning too!



Average return over 3 runs of the top-k candidates in an iterative batch generation approach

Reinforcement Learning in practice

- Very big, largely untapped potential!
- **Reward design and ability to simulate can be crucial**
- **Need to consider specifics of the problem**

- Great opportunity to improve existing algorithms!
- **Sample efficiency of RL needs to be improved**